Integral equation for inhomogeneous condensed bosons generalizing the Gross-Pitaevskii differential equation

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We give here the derivation of a Gross-Pitaevskii–type equation for inhomogeneous condensed bosons. Instead of the original Gross-Pitaevskii differential equation, we obtain an integral equation that implies less restrictive assumptions than are made in the very recent study of Pieri and Strinati [Phys. Rev. Lett. **91**, 030401 (2003)]. In particular, the Thomas-Fermi approximation and the restriction to small spatial variations of the order parameter invoked in their study are avoided.

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In a very stimulating recent contribution, Pieri and Strinati (referred to as PS below) [1] have 'derived' the non-linear Gross-Pitaevskii differential equation for condensed bosons by taking as their starting point the Bogoliubov-de Gennes equation for superfluid fermions.

The purpose of this Brief Report is to demonstrate that one can generalize the zero-temperature differential Gross-Pitaevskii equation while remaining within the original framework of PS, an integral equation formulation then resulting. The framework of PS is provided by the coupled integral equations involving Green functions G_{21}, G_{11} and $\tilde{G}_\circ$. The equations are:

$$G_{11}(\mathbf{r},\mathbf{r}';\omega_s) = \tilde{G}_\circ(\mathbf{r},\mathbf{r}';\omega_s) + \int d\mathbf{r}''\tilde{G}_\circ(\mathbf{r},\mathbf{r}'';\omega_s) \times\Delta(\mathbf{r}'')G_{21}(\mathbf{r}'',\mathbf{r}';\omega_s), \quad (1a)$$

$$G_{21}(\mathbf{r},\mathbf{r}';\omega_s) = -\int d\mathbf{r}''\tilde{G}_\circ(\mathbf{r}'',\mathbf{r};-\omega_s) \times\Delta^*(\mathbf{r}'')G_{11}(\mathbf{r}'',\mathbf{r}';\omega_s), \quad (1b)$$

where $\omega_s = (2s+1)\pi/\beta$ (s is an integer) is a fermionic Matsubara frequency, $\beta = 1/k_{\rm B}T$, G_{11} is the normal and G_{21} is the anomalous single-particle Green function. The third Green function appearing in Eqs. (1), namely $\tilde{G}_\circ$, satisfies the equation

$$[i\omega_s - H(\mathbf{r})]\tilde{G}_\circ(\mathbf{r},\mathbf{r}';\omega_s) = \delta(\mathbf{r}-\mathbf{r}'), \quad (2)$$

where the single-particle Hamiltonian $H(\mathbf{r})$ is defined by:

$$H(\mathbf{r}) = -\frac{\nabla^2}{2m} + V(\mathbf{r}) - \mu, \quad (3)$$

μ being the Fermionic chemical potential. As PS stress, Eqs. (1), when taken together with the self-consistency equation for the gap function:

$$\Delta^*(\mathbf{r}) = \frac{V_0}{\beta}\sum_s G_{21}(\mathbf{r},\mathbf{r};\omega_s), \quad (4)$$

are entirely equivalent to the Bogoliubov-de Gennes equations that describe the behavior of superfluid fermions in the presence of an external potential. Equations (1–4) define what we have termed the original framework of the PS study. The constant $V_0 < 0$ entering Eq. (4) arises from the contact potential $V_0\delta(\mathbf{r}-\mathbf{r}')$ assumed by PS to act between fermions with opposite spins. We also retain here their use of the ratio $\Delta(\mathbf{r})/\mu$ as an expansion parameter which allows the rapid truncation of such series, which then leads for strong coupling to an integral equation for the gap function

$$-\frac{1}{V_0}\Delta^*(\mathbf{r}) = \int d\mathbf{r}_1\, Q(\mathbf{r},\mathbf{r}_1)\Delta^*(\mathbf{r}_1) + \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3\, R(\mathbf{r},\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \times\Delta^*(\mathbf{r}_1)\Delta(\mathbf{r}_2)\Delta^*(\mathbf{r}_3), \quad (5)$$

where R is written explicitly in terms of $\tilde{G}_\circ(\mathbf{r},\mathbf{r}_1;\omega_s)$ in Eq. (15) of PS. However, as will emerge below, it is the non-local kernel $Q(\mathbf{r},\mathbf{r}')$ which is at the heart of the present study. In terms of the Green function $\tilde{G}_\circ$ entering Eq. (2), $Q(\mathbf{r},\mathbf{r}')$ is given by [PS: Eq. (14)]:

$$Q(\mathbf{r},\mathbf{r}') = \frac{1}{\beta}\sum_s \tilde{G}_\circ(\mathbf{r}',\mathbf{r};-\omega_s)\tilde{G}_\circ(\mathbf{r}',\mathbf{r};\omega_s). \quad (6)$$

We take the integral equation (5) for the gap function as the starting point of this Brief Report. For our purposes below, it is then crucial to gain insight into the kernel Q in Eq. (6), and in particular to carry out the summation explicitly over the Matsubara frequencies ω_s.

To gain orientation, let us first perform this summation when the external potential $V(\mathbf{r})$ is set to zero in Eq. (2). Having achieved this summation, we shall present a general method to allow the sum over ω_s to be achieved for $V(\mathbf{r}) \neq 0$, using earlier work of Stoddart, Hilton and March [2].

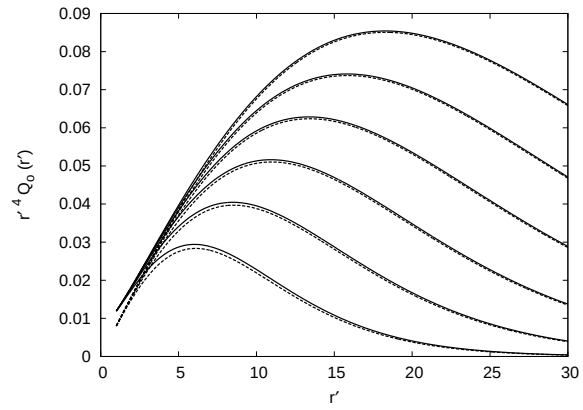

FIG. 1: Solid lines show $r'^4 Q_\circ(r')$, where $Q(r)$ is defined by Eq. (6), as a function of $r' = k_{\rm F} r$, for several temperatures, given by $\beta' = \beta\mu = 10 - 30$ (bottom to top). Dashed lines are the asymptotic expansion Eq. (8). Units are such that $k_{\rm F}^6/(4\mu) = 1$.

Returning to the explicit form of $Q(\mathbf{r}, \mathbf{r}_1)$ given in Eq. (6) above, it is natural to study first the translational invariant, free-electron limit of Eq. (6), say $Q_\circ(r)$, with $r = |\mathbf{r} - \mathbf{r}_1|$, which is obtained by 'switching off' the one-body potential $V(\mathbf{r})$. This amounts to replacing $\tilde{G}_\circ$ in Eq. (6) with the free-electron Green function $G_\circ$. For the Fourier transform of $Q_\circ(r)$, we formally find

$$\hat{Q}_\circ(k) = \int \frac{d\mathbf{k}'}{(2\pi)^3} \frac{1 - n_{\rm F}(\xi_{\mathbf{k}-\mathbf{k}'}) - n_{\rm F}(\xi_{\mathbf{k}'})}{\xi_{\mathbf{k}-\mathbf{k}'} + \xi_{\mathbf{k}'}}, \qquad (7)$$

where $\xi_{\mathbf{k}} = k^2/2m - \mu$ and $n_{\rm F}(\xi)$ is the Fermi-Dirac distribution function. However, it should be noted that, in three dimensions, Eq. (7) contains a divergent contribution at large wave-numbers, which implies a divergent behavior of $Q_\circ(r)$ at small distances r. Indeed, we find the asymptotic expansion (see also Ref. [3]):

$$\frac{4\mu}{k_{\rm F}^6} Q_\circ(r) \sim \frac{1}{4\pi^2} \frac{1}{r'^2 \beta'} \frac{1}{\sinh a}, \quad \beta' \gg 1, \qquad (8)$$

where $r' = k_{\rm F} r$, $k_{\rm F}$ is the Fermi wave-number, defined by $\mu = k_{\rm F}^2/2m$, $\beta' = \beta\mu$, and $a = r'\pi/\beta'$. Fig. 1 shows then our numerical results for $r'^4 Q_\circ(r')$, as a function of r', for several temperatures ($\beta' = 10 - 30$).

Following Stoddart *et al.* [2], the canonical density matrix $C(\mathbf{r}, \mathbf{r}', \beta)$ is defined by

$$C(\mathbf{r}, \mathbf{r}', \beta) = \sum_i \psi_i(\mathbf{r}) \psi_i^*(\mathbf{r}') e^{-\beta\epsilon_i}, \qquad (9)$$

where $\beta = 1/k_{\rm B}T$. Within the perturbative approach of March and Murray [4, 5], with plane waves as the unperturbed solution, the canonical density matrix can then be written to all orders in the external potential $V(\mathbf{r})$ in terms of the free-particle canonical density matrix given by

$$C_0(z, \beta) = (2\pi\beta)^{-3/2} \exp(-z^2/2\beta), \qquad (10)$$

as

$$C(\mathbf{r}, \mathbf{r}_0, \beta) = \int_0^\infty dz\, z\, C_0(z, \beta) f(z, \mathbf{r}, \mathbf{r}_0), \qquad (11)$$

where f satisfies the integral equation [2]:

$$f(z, \mathbf{r}, \mathbf{r}_0) = \frac{1}{z}\delta(z - |\mathbf{r} - \mathbf{r}_0|) - \int d\mathbf{r}_1 \frac{V(\mathbf{r}_1)}{2\pi|\mathbf{r} - \mathbf{r}_1|} \times f(z - |\mathbf{r} - \mathbf{r}_1|, \mathbf{r}_1, \mathbf{r}_0). \qquad (12)$$

The desired Green function $\tilde{G}_\circ$ is then to be obtained from f entering Eqs. (11) and (12) as [2]

$$\tilde{G}_\circ(\mathbf{r}, \mathbf{r}_1; k) = \int_0^\infty dz\, z\, \bar{G}_\circ(z; k) f(z, \mathbf{r}, \mathbf{r}_1), \qquad (13)$$

where

$$\bar{G}_\circ(z; k) = \frac{e^{ikz}}{4\pi z}. \qquad (14)$$

One may also take advantage of the expression in Eq. (13) of $\tilde{G}_\circ$ in terms of $\bar{G}_\circ$ to rewrite the kernel $Q(\mathbf{r}, \mathbf{r}_1)$ defined by Eq. (6) as

$$Q(\mathbf{r}, \mathbf{r}_1) = \int_0^\infty dz_1\, dz_2\, z_1\, z_2\, f(z_1, \mathbf{r}_1, \mathbf{r}) f(z_2, \mathbf{r}_1, \mathbf{r}) Q_\circ(z_1, z_2), \qquad (15)$$

where the Fourier transform of $Q_\circ(z_1, z_2)$ is given by

$$\hat{Q}_\circ(\mathbf{k}_1, \mathbf{k}_2) = \frac{1 - n_{\rm F}(\xi_{\mathbf{k}_1}) - n_{\rm F}(\xi_{\mathbf{k}_2})}{\xi_{\mathbf{k}_1} + \xi_{\mathbf{k}_2}}. \qquad (16)$$

Hence, the sum over Matsubara frequencies has still been carried out in the presence of an external potential $V(\mathbf{r})$ entering Eq. (12) for the function f.

Because of current interest in harmonic confinement in magnetic traps at low temperatures, let us illustrate the rather formal Eqs. (11) and (12) when the external potential $V(\mathbf{r})$ has the explicit isotropic harmonic oscillator form in three dimensions, namely

$$V(\mathbf{r}) = \frac{1}{2} m\omega^2 r^2. \qquad (17)$$

Following the pioneering work of Sondheimer and Wilson [6] on free electrons in a magnetic field, the diagonal element $C(\mathbf{r}, \mathbf{r}, \beta)$ when $V(\mathbf{r})$ is given by Eq. (17) takes the form (see *e.g.* [7], p. 27; see also [8])

$$C(\mathbf{r}, \mathbf{r}, \beta) = \left(\frac{m}{2\pi\hbar}\right)^{3/2} \left(\frac{\omega}{\sinh \hbar\omega\beta}\right)^{3/2} \times \exp\left(-\frac{m}{\hbar}\omega r^2 \tanh \frac{1}{2}\hbar\omega\beta\right), \qquad (18)$$

which is the so-called Slater sum of quantum chemistry (Fig. 2).

From Eqs. (10) and (11), performing the substitution $t = z^2/2$, it then follows that $f(z, \mathbf{r}, \mathbf{r}_0)$ can be expressed as the inverse Laplace transform

$$f(z, \mathbf{r}, \mathbf{r}_0) = (2\pi)^{3/2} \mathcal{L}^{-1}\left[s^{-3/2} C(\mathbf{r}, \mathbf{r}_0, s^{-1})\right] \qquad (19)$$

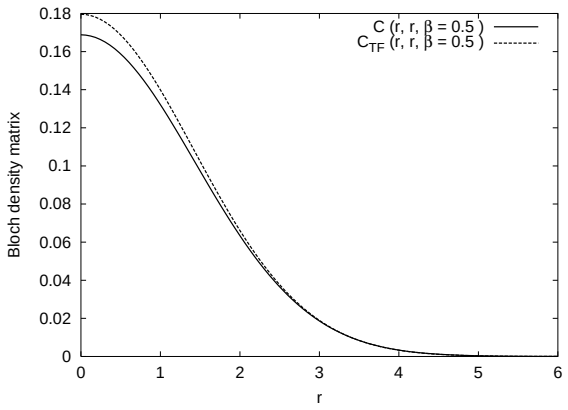

FIG. 2: Shows diagonal element of the canonical density matrix $C(\mathbf{r},\mathbf{r},\beta)$, Eq. (18), and its Thomas-Fermi approximation, Eq. (20), as a function of r, for $\beta = 0.5$. Energies are in units of $\hbar\omega$, while lengths are in units of $(\hbar/m\omega)^{1/2}$.

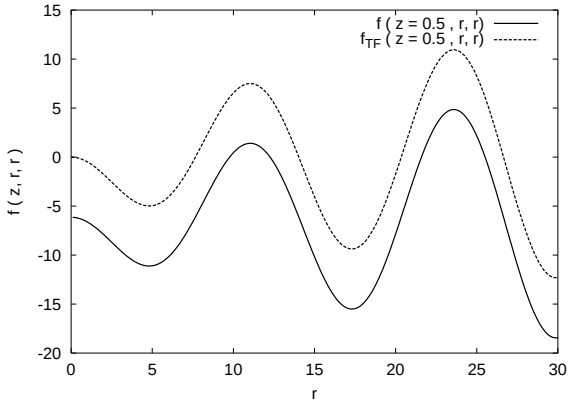

FIG. 3: Shows diagonal $f(z,\mathbf{r},\mathbf{r})$ corresponding to the harmonic potential, as given by the inverse Laplace transform, Eq. (19), as well as the regular part of its Thomas-Fermi approximation, Eq. (21), as a function of r, for fixed $z = 0.5$. Units as in Fig. 2.

where (t,s) are conjugate variables with respect to the Laplace transform.

Within the Thomas-Fermi (TF) approximation, we take:

$$C_{\rm TF}(\mathbf{r},\mathbf{r},\beta) = \frac{1}{(2\pi\beta)^{3/2}}\exp[-\beta V(\mathbf{r})], \qquad (20)$$

which is plotted also in Fig. 2 for $V(\mathbf{r})$ given by Eq. (17). For the value of β shown, the TF form Eq. (20) is seen to be a useful approximation to the exact result, Eq. (18). Inserting Eq. (20) into Eq. (19) we find

$$f_{\rm TF}(z,\mathbf{r},\mathbf{r}) = \frac{\delta(z)}{z} - \frac{\sqrt{2V(\mathbf{r})}}{z}J_1[\sqrt{2V(\mathbf{r})}z], \qquad (21)$$

where J_1 denotes the Bessel function of the first kind and order one.

Fig. 3 shows $f(z,\mathbf{r},\mathbf{r})$ as a function of r for fixed z, as obtained by numerically performing the inverse Laplace transform in Eq. (19) for the harmonic potential case. The regular contribution to the analytic result for the Thomas-Fermi approximation, Eq. (21), is also plotted for comparison. The similarity in shape between approximate and (numerically) exact results for this harmonic confinement model seems to us rather remarkable. After this model test of a TF-like approximation invoked by PS, we return to the general case, based on the exact result Eq. (15) for the kernel $Q(\mathbf{r},\mathbf{r}_1)$.

Then, we invert the argument of PS but still use a further essential assumption of their study, namely that the condensate wave function $\Phi(\mathbf{r})$ entering the Gross-Pitaevskii equation is related to the gap function $\Delta(\mathbf{r})$ by

$$\Phi(\mathbf{r}) = \left(\frac{m^2 a_{\rm F}}{8\pi}\right)^{1/2}\Delta(\mathbf{r}) \equiv k\Delta(\mathbf{r}). \qquad (22)$$

Here, in the strong coupling limit, and following PS, $a_{\rm F} \sim (2m|\mu|)^{-1/2}$ represents the characteristic length scale for the non-interacting Green function $G_\circ$, equal to $\tilde{G}_\circ$ above when $V(\mathbf{r})$ is put equal to zero.

Given the validity of this PS assumption, Eq. (22), we then rewrite Eq. (5) as an equation for $\Phi(\mathbf{r})$:

$$\begin{aligned} -\frac{1}{V_0}\Phi^*(\mathbf{r}) \;&=\; \int d\mathbf{r}_1\, Q(\mathbf{r},\mathbf{r}_1)\Phi^*(\mathbf{r}_1) \\ &\quad + \frac{1}{k^2}\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3\, R(\mathbf{r},\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \\ &\quad \times\Phi^*(\mathbf{r}_1)\Phi(\mathbf{r}_2)\Phi^*(\mathbf{r}_3). \end{aligned} \qquad (23)$$

This then is the proposed generalization of the Gross-Pitaevskii equation, but with $Q(\mathbf{r},\mathbf{r}_1)$ to be calculated more accurately than by the Thomas-Fermi–like assumption of Pieri and Strinati [1], via Eqs. (15) and (12).

While Eq. (23) is a direct consequence of the above arguments, it remains an expansion in Φ, in suitable reduced form. Therefore, a first attempt to simplify this Eq. (23) is to retain the approximation given by the Pieri-Strinati approach in the 'smallest' term involving $O(\Phi^3)$ on the right-hand side of the basic Eq. (23). Thus one reaches the (still non-local) equation for the condensate wave function $\Phi(\mathbf{r})$:

$$\begin{aligned} -\frac{1}{V_0}\Phi^*(\mathbf{r}) \;&=\; \int d\mathbf{r}_1\, Q(\mathbf{r},\mathbf{r}_1)\Phi(\mathbf{r}_1) \\ &\quad - \frac{m a_{\rm F}^2}{2}|\Phi(\mathbf{r})|^2\Phi(\mathbf{r}). \end{aligned} \qquad (24)$$

For sufficiently small spatial variations in the condensate wave function $\Phi(\mathbf{r})$ in Eq. (24), the basic nonlocality can be removed by Taylor expanding $\Phi(\mathbf{r}_1)$ around the position $\mathbf{r}$ in the integral term. This then characterizes the problem in terms of 'partial moments' of the kernel $Q(\mathbf{r},\mathbf{r}_1)$, namely $\int Q(\mathbf{r},\mathbf{r}_1)d\mathbf{r}_1$ and $\int Q(\mathbf{r},\mathbf{r}_1)|\mathbf{r}-\mathbf{r}_1|^2 d\mathbf{r}_1$. Such partial moments then enter the original Gross-Pitaevskii equation, as stressed by PS.

In summary, we propose the retention of the non-local kernel $Q(\mathbf{r},\mathbf{r}_1)$ as in Eq. (23) above, since the sum over

Matsubara frequencies in Eq. (6) has been performed in Eq. (15), which is a central result of the present study. However, in the terms of $O(\Phi^3)$ in Eq. (23), a sensible starting point is to follow the PS approximation displayed in Eq. (24).

As to future directions, evaluation of the non-local kernel in Eq. (15) for other external potentials than the harmonic case in Eq. (17) is of obvious interest. For this latter model, though our Fig. 3 considers the diagonal element of $f(z, \mathbf{r}, \mathbf{r}_1)$, the off-diagonal form of $C(\mathbf{r}, \mathbf{r}_1, \beta)$ is known [8], and numerical Laplace inversion to obtain $f(z, \mathbf{r}, \mathbf{r}_1)$ is entirely feasible. Then $Q(\mathbf{r}, \mathbf{r}_1)$ can be obtained, though of course numerically.

The Gross-Pitaevskii equation is valid in the strong-coupling limit of superfluidity. It has to be stressed that in the weak coupling limit one can also derive a Ginzburg-Landau equation starting from the Bogoliubov-de Gennes equations. We note specifically in this context that the derivation of the Ginzburg-Landau equation in the weak-coupling limit for the harmonic trap was presented by Baranov and Petrov [9]. The results presented in this Brief Report are also relevant to the weak-coupling limit of superfluidity.

Finally, we should mention the very recent discussions of the foundations of the Gross-Pitaevskii equation by Leggett [10]. He concludes that there is no correlated many-body wave-function underlying their original equation. It will be interesting for the future to know whether the non-local versions of Eqs. (23) and (24) proposed here are still subject to this limitation.

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